PHY 102 Modern Physics Mid-Term Exam I
Date: January 29, 2013 **Name: ___________________________________**

1. (20 points) There are four particles moving in a three dimensional space as described below. Write the Hamiltonian (H = T + U) for the particles. Determine whether the Hamiltonian of the particles are translationally and/or rotationally invariant and explain why. Based on this information, determine whether linear or angular momentum is conserved.

(1) (4 points) A free particle with energy E moving in a 3 dimensional space.

Hamiltonian =

$$-\frac{\hbar^2}{2m}\nabla^2$$

Translational invariance:

Since the potential does not depend on position (x,y,z), the H of Particle A is translationally invariant. That is

$$H(x,y,z) = H(x+a, y+b, z+c) = -\frac{\hbar^2}{2m}\nabla^2$$

Rotational invariance:

Since the potential does not depend on position or angle, the H of Particle A is rotationally invariant. That is

$$H(r,\theta,\phi) = H(r,\theta+b,\phi+c) = -\frac{\hbar^2}{2m}\nabla^2$$

Momentum conservation

Since H is trsnalationally invariant, the linear momentum is conserved.
Since H is not rotationally invariant, the angular momentum is not conserved.

(2) (4 points) An electron moving around a proton (hydrogen atom)

Hamiltonian =

$$-\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r} \quad OR \quad -\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{\sqrt{x^2+y^2+z^2}}$$

Translational invariance:

Since the potential depends on position (x,y,z), the H is translationally not invariant. That is

$$H(x,y,z) = -\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{\sqrt{x^2+y^2+z^2}}$$

$$H(x+a,y+b,z+c) = -\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{\sqrt{(x+a)^2+(y+b)^2+(z+c)^2}}$$

Rotational invariance:

Since the potential does not depend on $\theta\ or\ \phi$, the H is rotationally invariant. That is,

$$H(r,\theta,\phi) = H(r,\theta+b,\phi+c) = -\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}$$

Momentum conservation

Since H is trsnalationally not invariant, the linear momentum is not conserved.
Since H is rotationally invariant, the angular momentum is conserved.

(3) (4 points) A particle moving inside a spherical hollow of which radius is L.

Hamiltonian =

$$H = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})$$

Where $U(\vec{r}) = \begin{cases} 0, & |\vec{r}| \le L \\ \infty, & \text{otherwise} \end{cases}$

Translational invariance:

Since the potential depends on position, the H is not translationally invariant. That is

$$H(x, y, z) = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}) \text{ Where } U(\vec{r}) = \begin{cases} 0, & |\vec{r}| \le L \\ \infty, & \text{otherwise} \end{cases}$$

$$H(x + a, y + b, z + c) = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r}) \text{ Where}$$
$$U(\vec{r}) = \begin{cases} 0, & \sqrt{(x+a)^2 + (y+b)^2 + (z+c)^2} \le L \\ & \infty, \ \text{otherwise} \end{cases}$$

Rotational invariance:

Since the potential does not depend on angles, the H is rotationally invariant. That is

$$H(r, \theta, \phi) = H(r, \theta + b, \phi + c)$$

Momentum conservation

Since H is trsnalationally not invariant, the linear momentum is not conserved.
Since H is rotationally invariant, the angular momentum is conserved.

(4) (4 points) A three dimensional harmonic oscillator

Hamiltonian =

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}kr^2$$

Translational invariance:

Since the potential depends on position, the H is not translaitonally invariant. That is.

$$H(x, y, z) = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}k(x^2 + y^2 + z^2)$$

$$H(x + a, y + b, z + c) = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}k[(x + a)^2 + (y + b)^2 + (z + c)^2]$$

Rotational invariance:

Since the potential does not depend on angles, the H is rotationally invariant. That is

$$H(r, \theta, \phi) = H(r, \theta + b, \phi + c) = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}kr^2$$

Momentum conservation

Since H is trsnalationally not invariant, the linear momentum is not conserved.
Since H is rotationally invariant, the angular momentum is conserved

(5) (2 points) Which particles' angular motions might be described using spherical harmonics ($Y_l^{m_l}$)?

Particles of which Hamiltonian are rotationally invariant can have spherical harmonics to describe their angular motions. Thus, all four particles in the problem 1 can have spherical harmonics.

2.(10 points) Identify different quantum states that are possible for an electron in the 4d orbital. Consider both spin and orbital angular momentum.

(1) (5 points) When a strong magnetic field is present (Hint: Use (n, l, m_l, m_s))

n	l	m_l	m_s
4	2	-2	+1/2
			-1/2
		-1	+1/2
			-1/2
		0	+1/2
			-1/2
		1	+1/2
			-1/2
		2	+1/2
			-1/2

A total of 10 states

(2) (5 points) When a weak magnetic field is present (Hint: Use (n, l, j, m_j))

n	l	j	m_j
4	2	5/2	5/2
			3/2
			1/2
			-1/2
			-3/2
			-5/2
		3/2	3/2
			1/2
			-1/2
			-3/2

A total of 10 states

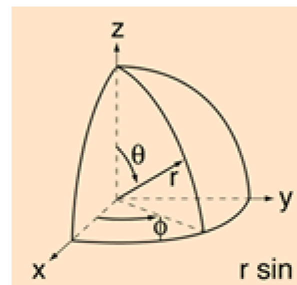
3. (15 points+ Extra 5 points) Consider a hydrogen atom. In this problem, you will obtain selection rules associated with the quantum number m_l. In general, selection rules can be obtained by examining the following integral:

$$\int_{-\infty}^{\infty} u\psi_{n,l,m_l}{}^{*}\,\psi_{n\prime,l\prime,m_l\prime}dV \quad where\ u = x, y, or\ z$$

For allowed transitions, this integral should not be zero.

(a) (2 points) In the spherical coordinate system shown in the figure, how $u\ (i.e. x, y, and\ z)$ and *dV* can be expressed?

$$x = rsin\theta cos\phi$$
$$y = r\ sin\theta sin\ \phi$$
$$z = rcos\theta$$
$$dV = r^2 sin\theta drd\theta d\phi$$



(b) (2 points) Write an expression for the expected x value in spherical coordinate system:

$$< x > = \int_{-\infty}^{\infty} x\psi_{n,l,m_l}{}^{*}\,\psi_{n\prime,l\prime,m_l\prime}dV =$$

$$= \int_{-\infty}^{\infty} rsin\theta cos\phi\ \psi_{n,l,m_l}{}^{*}\,\psi_{n\prime,l\prime,m_l\prime}r^2 sin\theta drd\theta d\phi$$

$$= \int_{-\infty}^{\infty} r^3 sin^2\theta cos\phi\ \psi_{n,l,m_l}{}^{*}\,\psi_{n\prime,l\prime,m_l\prime}drd\theta d\phi$$

(c) (3 points) Apply the Separation of Variables method shown below, express <x> in terms of three integral products.

$$\psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r)\Theta_{l,m_l}(\theta)\Phi_{m_l}(\phi)$$

$$= \int_0^{\infty} r^3 R_{n,l}{}^{*}(r)R_{n\prime,l\prime}(r)dr \int_0^{\pi} \Theta_{l,m_l}{}^{*}(\theta)\Theta_{l\prime,m_l\prime}(\theta)\ sin^2\theta\ d\theta \int_0^{2\pi} \Phi_{m_l}{}^{*}(\phi)\ \Phi_{m_l\prime}(\phi)cos\phi\ d\phi$$

(d) (3 points) From (c), we know that the integral part concerning ϕ is

$$\int_0^{2\pi} \Phi_{m_l}{}^* \Phi_{m_l'} cos\phi d\phi$$

Consider the following:

$$\begin{cases} \Phi_{m_l} = \dfrac{1}{\sqrt{2\pi}} e^{im_l\phi} \\ cos\phi = \dfrac{e^{i\phi} + e^{-i\phi}}{2} \end{cases}$$

Re-express the integral part concerning ϕ

$$\int_0^{2\pi} \Phi_{m_l}{}^* \Phi_{m_l'} cos\phi d\phi = \frac{1}{2\pi} \int_0^{2\pi} e^{i(m_l - m_l')\phi} \left(\frac{e^{i\phi} + e^{-i\phi}}{2} \right) d\phi$$

$$= \frac{1}{4\pi} \int_0^{2\pi} e^{i(m_l - m_l')\phi} \left(e^{i\phi} + e^{-i\phi} \right) d\phi$$

$$= \frac{1}{4\pi} \int_0^{2\pi} e^{i(m_l - m_l' + 1)\phi} d\phi + \frac{1}{4\pi} \int_0^{2\pi} e^{i(m_l - m_l' - 1)\phi} d\phi$$

(e) (5 points) From (d) prove that the selection rule concerning Δm_l should be $\Delta m_l = \pm 1$.

For the integral in (d) to have a finite value,

$$m_l - m_l' + 1 = 0 \;\; OR \; m_l - m_l' - 1 = 0$$

That is,

$$\Delta m_l = m_l{}' - m_l = \pm 1$$

[OPTIONAL: EXTRA 5 points]

(f) Obtain

$$< z > = \int_{-\infty}^{\infty} z\psi_{n,l,m_l}{}^{*}\,\psi_{n\prime,l\prime,m_l\prime}dV$$

$$= \int_{-\infty}^{\infty} rcos\theta cos\phi\;\psi_{n,l,m_l}{}^{*}\,\psi_{n\prime,l\prime,m_l\prime}r^2 sin\theta drd\theta d\phi$$

$$= \int_{-\infty}^{\infty} r^3 cos\theta sin\theta\;\psi_{n,l,m_l}{}^{*}\,\psi_{n\prime,l\prime,m_l\prime}drd\theta d\phi$$

$$= \int_0^{\infty} r^3 R_{n,l}{}^{*}(r)R_{n\prime,l\prime}(r)dr \int_0^{\pi}\Theta_{l,m_l}{}^{*}(\theta)\Theta_{l\prime,m_{l\prime}}(\theta) \quad cos\theta sin\theta d\theta \int_0^{2\pi}\Phi_{m_l}{}^{*}(\phi)\,\Phi_{m_l\prime}(\phi)\,d\phi$$

(g) repeat (d) for <z> and show that another selection rule should be $\Delta m_l = 0$.

$$\int_0^{2\pi}\Phi_{m_l}{}^{*}\Phi_{m_l\prime}cos\phi d\phi = \frac{1}{2\pi}\int_0^{2\pi} e^{i(m_l - m_l')\phi}d\phi$$

For the integral in (d) to have a finite value,

$$m_l - m_l' = 0$$

That is,

$$\Delta m_l = m_l{}' - m_l = 0$$

4. (15 points)To describe a many-electron state, an elementary way is to use the Slater Determinant. Consider putting two electrons in 1s shell in He. The Slater determinant wave function is given by

$$\psi(x_1, x_2, u_1, u_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_{1s}(x_1) \uparrow_1 & \psi_{1s}(x_1) \downarrow_1 \\ \psi_{1s}(x_2) \uparrow_2 & \psi_{1s}(x_2) \downarrow_2 \end{vmatrix}$$

where

- $\uparrow_1$ means the spin wave function where the "spin coordinate" $u_1 \equiv m_{s,1} = \frac{1}{2}$
- $\downarrow_1$ means the spin wave function $u_1 \equiv m_{s,1} = -\frac{1}{2}$.
- x_1, u_1 are the spatial and spin coordinates of particle 1 and x_2, u_2 are those of particle 2.
- The spin coordinate for an electron is binary by nature: $u_1 = \frac{1}{2}$ or $-\frac{1}{2}$ and $u_2 = \frac{1}{2}$ or $-\frac{1}{2}$.
- Note that the determinant of a 2 x 2 matrix is $\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$

(a) (4 points) Determine whether $\psi(x_1, x_2, u_1, u_2)$ is symmetric or anti-symmetric under the spatial state exchange.

Two spatial states are in the same 1s state. Therefore, the spatial state exchange means $\psi_{1s} \leftrightarrow \psi_{1s}$

If this occurs, there is no change in the determinant shown above.

$$SpatialEXCH[\psi(x_1, x_2, u_1, u_2)] = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_{1s}(x_1) \uparrow_1 & \psi_{1s}(x_1) \downarrow_1 \\ \psi_{1s}(x_2) \uparrow_2 & \psi_{1s}(x_2) \downarrow_2 \end{vmatrix}$$

$$= \frac{1}{\sqrt{2}}[\psi_{1s}(x_1) \uparrow_1 \psi_{1s}(x_2) \downarrow_2 - \psi_{1s}(x_1) \downarrow_1 \psi_{1s}(x_2) \uparrow_2] = \psi(x_1, x_2, u_1, u_2)$$

➔ Symmetric under the spatial state exchange

Alternatively,

$$\begin{aligned} \psi(x_2, x_1, u_1, u_2) &= \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_{1s}(x_2) \uparrow_1 & \psi_{1s}(x_2) \downarrow_1 \\ \psi_{1s}(x_1) \uparrow_2 & \psi_{1s}(x_1) \downarrow_2 \end{vmatrix} \\ &= \frac{1}{\sqrt{2}}[\psi_{1s}(x_2) \uparrow_1 \psi_{1s}(x_1) \downarrow_2 - \psi_{1s}(x_2) \downarrow_1 \psi_{1s}(x_1) \uparrow_2] \\ &= \frac{1}{\sqrt{2}}[\psi_{1s}(x_1) \uparrow_1 \psi_{1s}(x_2) \downarrow_2 - \psi_{1s}(x_1) \downarrow_1 \psi_{1s}(x_2) \uparrow_2] = \psi(x_1, x_2, u_1, u_2) \end{aligned}$$

(b) (4 points) Determine whether $\psi(x_1, x_2, u_1, u_2)$ is symmetric or anti-symmetric under the spin exchange.

Two spin states are in opposite spins. Therefore, the spin state exchange means $\uparrow \leftrightarrow \downarrow$

Then,

$$SpinEXCH[\psi(x_1, x_2, u_1, u_2)] = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_{1s}(x_1) \downarrow_1 & \psi_{1s}(x_1) \uparrow_1 \\ \psi_{1s}(x_2) \downarrow_2 & \psi_{1s}(x_2) \uparrow_2 \end{vmatrix}$$

$$= \frac{1}{\sqrt{2}}[\psi_{1s}(x_1) \downarrow_1 \psi_{1s}(x_2) \uparrow_2 - \psi_{1s}(x_1) \uparrow_1 \psi_{1s}(x_2) \downarrow_2] = -\psi(x_1, x_2, u_1, u_2)$$

➔ Anti-symmetric under the spin state exchange

Alternatively,

$$\psi(x_1, x_2, u_2, u_1) = \frac{1}{\sqrt{2}}\begin{vmatrix}\psi_{1s}(x_1)\uparrow_2 & \psi_{1s}(x_1)\downarrow_2 \\ \psi_{1s}(x_2)\uparrow_1 & \psi_{1s}(x_2)\downarrow_1\end{vmatrix}$$
$$= \frac{1}{\sqrt{2}}[\psi_{1s}(x_1)\uparrow_2 \psi_{1s}(x_2)\downarrow_1 - \psi_{1s}(x_1)\downarrow_2 \psi_{1s}(x_2)\uparrow_1]$$
$$= \frac{1}{\sqrt{2}}[\psi_{1s}(x_1)\downarrow_1 \psi_{1s}(x_2)\uparrow_2 - \psi_{1s}(x_1)\uparrow_1 \psi_{1s}(x_2)\downarrow_2] = -\psi(x_1, x_2, u_1, u_2)$$

(c) (4 points) Determine whether $\psi(x_1, x_2, u_1, u_2)$ is symmetric or anti-symmetric under the spin and spatial state exchange.

Under both spatial and spin state exchange, $both\ \psi_{1s} \leftrightarrow \psi_{1s}\ \ and\ \uparrow\leftrightarrow\downarrow\ \ occur$

$$Space\&SpinEXCH[\psi(x_1, x_2, u_1, u_2)] = \frac{1}{\sqrt{2}}\begin{vmatrix}\psi_{1s}(x_1)\downarrow_1 & \psi_{1s}(x_1)\uparrow_1 \\ \psi_{1s}(x_2)\downarrow_2 & \psi_{1s}(x_2)\uparrow_2\end{vmatrix}$$
$$= \frac{1}{\sqrt{2}}[\psi_{1s}(x_1)\downarrow_1 \psi_{1s}(x_2)\uparrow_2 - \psi_{1s}(x_1)\uparrow_1 \psi_{1s}(x_2)\downarrow_2] = -\psi(x_1, x_2, u_1, u_2)$$

➔ Antisymmetric under both spatial and spin state exchange

Alternatively,

$$\psi(x_2, x_1, u_2, u_1) = \frac{1}{\sqrt{2}}\begin{vmatrix}\psi_{1s}(x_2)\uparrow_2 & \psi_{1s}(x_2)\downarrow_2 \\ \psi_{1s}(x_1)\uparrow_1 & \psi_{1s}(x_1)\downarrow_1\end{vmatrix}$$
$$= \frac{1}{\sqrt{2}}[\psi_{1s}(x_2)\uparrow_2 \psi_{1s}(x_1)\downarrow_1 - \psi_{1s}(x_2)\downarrow_2 \psi_{1s}(x_1)\uparrow_1]$$
$$= \frac{1}{\sqrt{2}}[\psi_{1s}(x_1)\downarrow_1 \psi_{1s}(x_2)\uparrow_2 - \psi_{1s}(x_1)\uparrow_1 \psi_{1s}(x_2)\downarrow_2] = -\psi(x_1, x_2, u_1, u_2)$$

(d) (3 points) [Consider this part from a more general point of view, possibly going beyond the wave function given above.] If both electrons are in the 1s shell, then which of the following spin arrangements are possible (choose one)
___ both spins up
_x__ one spin up and the other down
___ both spins down
Explain your answer using the Slater Determinant.

If both spins are up in the 1s shell:

$$\psi(x_1, x_2, u_1, u_2) = \frac{1}{\sqrt{2}}\begin{vmatrix}\psi_{1s}(x_1)\uparrow_1 & \psi_{1s}(x_1)\uparrow_1 \\ \psi_{1s}(x_2)\uparrow_2 & \psi_{1s}(x_2)\uparrow_2\end{vmatrix}$$
$$= \frac{1}{\sqrt{2}}[\psi_{1s}(x_1)\uparrow_1 \psi_{1s}(x_2)\uparrow_2 - \psi_{1s}(x_1)\uparrow_1 \psi_{1s}(x_2)\uparrow_2]$$
$$= \frac{1}{\sqrt{2}}[\psi_{1s}(x_1)\psi_{1s}(x_2)\uparrow_1\uparrow_2 - \psi_{1s}(x_1)\psi_{1s}(x_2)\uparrow_1\uparrow_2] = 0$$

The Slater determinant vanishes for such arrangement. It is impossible.
The same goes to the case when both spins are down.

5**. True/False Questions (10 points)** Determine whether each of the following statements is true or false. Then, briefly explain your answer.

(a) (3 points) Knowing the magnitude and the z-component of the angular momentum of an electron in the hydrogen atom does not violate uncertainty principle.

_x_ True ___ False

Explain your answer.

Because the x and the y components of the angular momentum are still unknown, the particle is not confined to a single plane. If the particle is confined to a single plane, the displacement of the particle along the axis perpendicular to the plane as well as the linear momentum along the axis will be zero, thus violating the uncertainty principle.

(b) (4 points) Anti-parallel spin arrangements in the same orbital are in general more stable than parallel spin arrangements if the orbital shell (e.g., 2p shell or 3d shell) is less than half full. ___ True _x_ False

Explain your answer.

The wave function of a system of electrons orbiting a nucleus should be antisymmetric under the particle exchange. The wave function is a product of the spatial state wave function and the spin state wave function. If the spin state wave function part has anti-parallel spin arrangements, then the spatial state function part should be symmetric. This means the electrons occupy the same orbital space, putting the electrons closer together than when electrons do not occupy the same orbital space. This increases energy due to repulsive Coulomb interactions between the negatively charged electrons.

(c) (3 points) Spin and orbital angular momentum of an electron is always coupled.

___ True _x_ False

Explain your answer.

In the presence of weak magnetic fields, the spin angular momentum and the orbital angular momentum are coupled. In the presence of strong magnetic fields, such coupling breaks, leading to the spin angular momentum and the orbital angular momentum to separately respond to the magnetic field.